National Aeronautics and Space Administration

NASA'S TECHNOLOGY INFUSION ROAD TOUR

Historically Black Colleges/Universities & Minority Serving Institutions

NEW MEXICO STATE UNIVERSITY

New Mexico Highlands University
AI/Machine Learning in Materials Science

Dr. Gil R. Gallegos

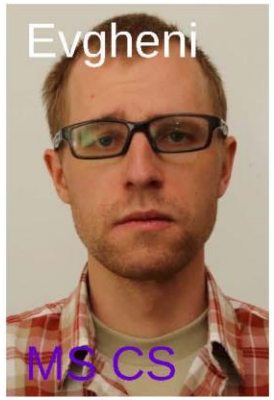
gil.gallegos@gmail.com

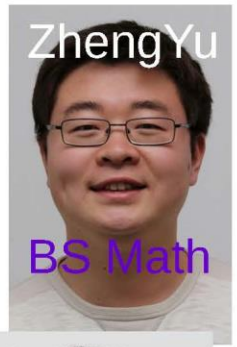
505-414-1562

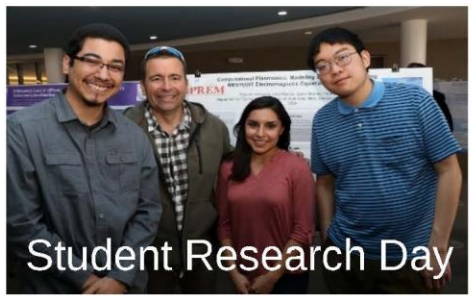
Date 8-13-19

Office of Small Business Mentor-Protégé Program

Research - Thrust 3b: Machine learning – artificial intelligence – material sciences







PREM-NSF Computer Science (Materials Science/Machine Learning Workflow)

Objective: *Characterization of biosensor morphology utilizing machine learning to predict resonant frequency of novel scanning electron microscope (SEM) images of random nanostar distributions.*

Step 1: Novel SEM image is pre-processed by Feature Identification Algorithm (FIA)
Step 2: Construct feature vector with features f_i, i=1,2,3,...m

X = **x1** = [f1 f2 f3...fm]
x2 = [f1 f2 f3...fm]
...
xn = [f1 f2 f3...fm]

= [Features]

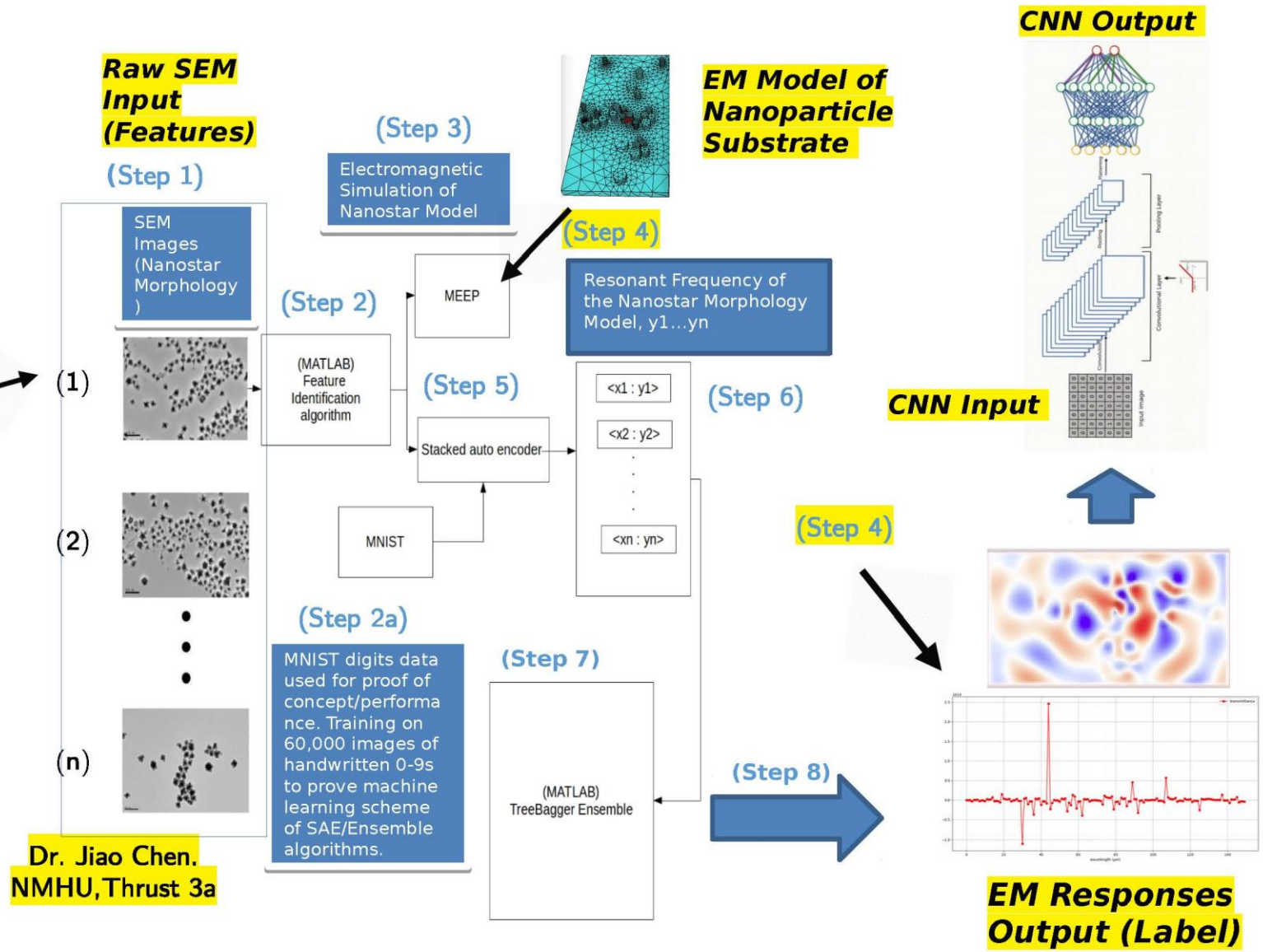
Step 3: Utilizing FIA information –construct electromagnetic models for MIT Electromagnetic Equation Propagation (MEEP) solver.

Step 4: Solver computes resonant frequency for SEM morphology, **y_i**, i=1,2,3...n

Step 5: Stacked Auto-Encoder (SAE) learns lower dimensional vector **hi** to represent **x_i** for i=1,2,3,...n
Step 6: New X is created from **h_i** and **y_i**

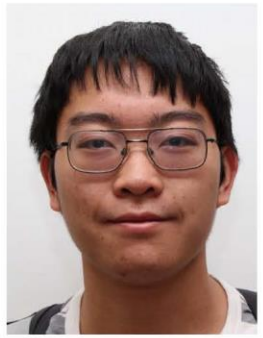
Step 7: Ensemble, machine learning algorithm uses **h_i** features and **y_i**, predictions to build prediction model for resonant frequency of SEM morphologies.

Step 8: Novel SEM image (not in training set) is then processed Steps 1 through 7. Resonant frequency is predicted (Excitation light wavelength now known)



Dr. Jiao Chen.
NMHU,Thrust 3a

Research - Project 2: *Generation of Machine Learning Output (Label) Images for Convolutional Neural Network (CNN) Training :Utilizing Ab Initio Electromagnetic (EM) Simulation of Nanoparticle Substrate Input (Features) from Scanning Electron Microscope (SEM) Images*

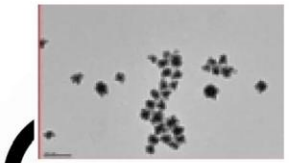


Henry Chung
BS CS, NMHU

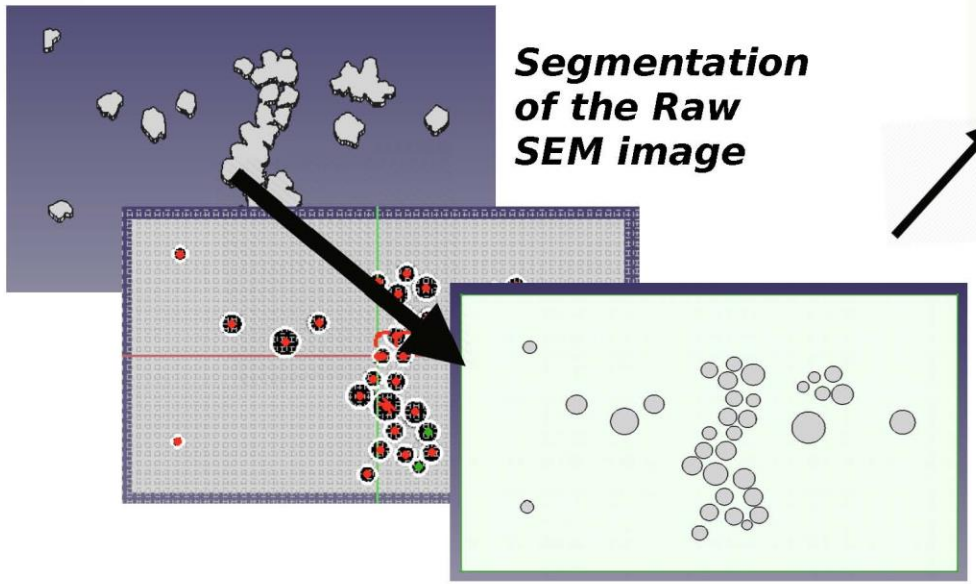
2nd Semester Graduate Student , MS CS, NMHU

Research:
Computational modeling/ simulation of metamaterials and AI/machine learning

Employment: PREM

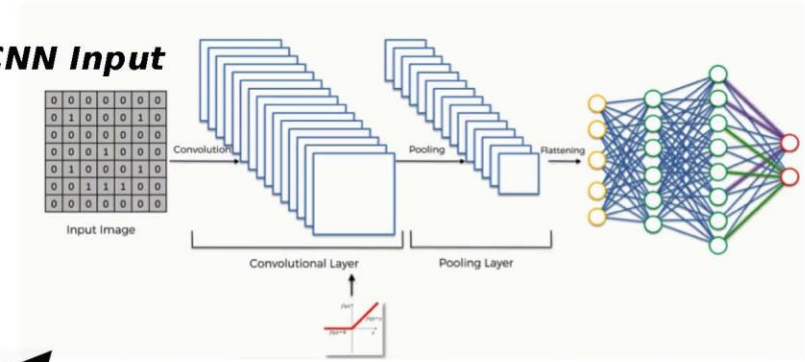


Raw SEM Input (Features)



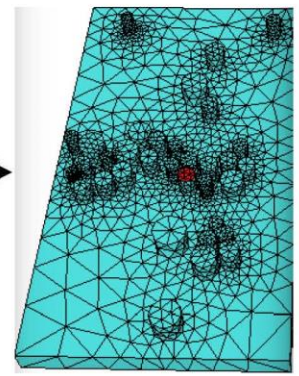
Segmentation of the Raw SEM image

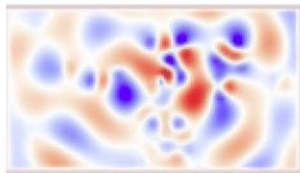
CNN Input



CNN Output

EM Model of Nanoparticle Substrate





EM Response Output (Labels)

Research - Project 3: *Predicting Atomization Energies Using Machine Learning And Principal Component Analysis (PCA)*

Fred Sena
BS CS, NMHU

3rd Semester Graduate Student , MS CS, NMHU

Research: Computational modeling/ simulation of metamaterials and AI/machine learning

Employment: LANL

- Machine Learning and Principal Component Analysis (PCA)

- Predict atomization energies of crystal structures

- Dataset containing over 7000 molecules

- Dataset contained over 500 features

- PCA is used to extract only the most important features

- Reduces the original feature set by nearly 70%

- The primary goal of this research is to improve the computational efficiency of the machine learning model, while ensuring the accuracy is not lost

```
model = Sequential()
model.add(Dense(256, activation=keras.activations.linear)),
model.add(Dense(128, activation=keras.activations.linear)),
model.add(Dense(64, activation=keras.activations.linear)),
model.add(Dropout(0.1)),
model.add(Dense(1, activation=keras.activations.linear))

model.compile(optimizer='adam',
              loss='mean_squared_error',
              metrics=['accuracy'])

model.fit(x_train, y_train, epochs=200)
model.evaluate(x_test, y_test)
y_pred = model.predict(x_test)
```

Python, KERAS , Neural Network Code Snippet

Network	Accuracy	Training Time	Dataset Shape
Neural Network (No PCA)	97.96%	67 Seconds	7165, 529
Neural Network (PCA)	97.87%	49 Seconds	7165, 160

Results

NEW MEXICO HIGHLANDS UNIVERSITY

ARMAS in Education

Achieving in Research, Math, And Science

Rosario Vasquez
BS CS, NMHU

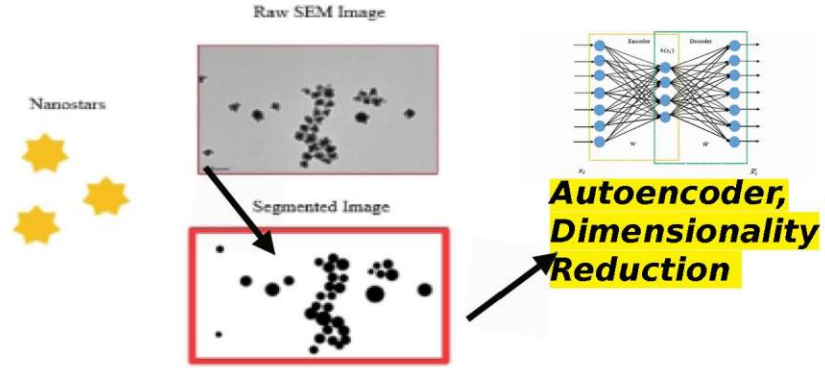
4th Semester Graduate Student , MS CS, NMHU

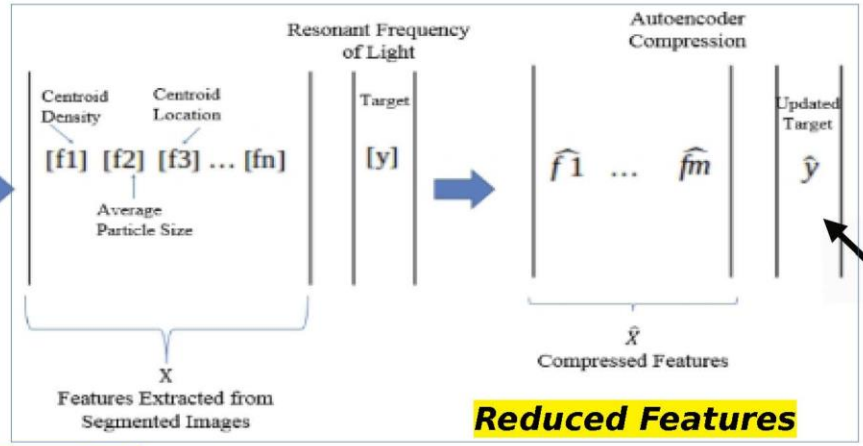
Research:
Computational modeling/ simulation of metamaterials and AI/machine learning

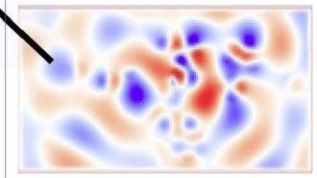
Employment: LANL

Research - Project 4:

Classification/Dimesionality Reduction (DR) Utilizing Autoencoders and Ensemble Learning







EM Response Output (Labels)

Current Research:

- Dimensionality reduction on MNIST data set to improve digit classification

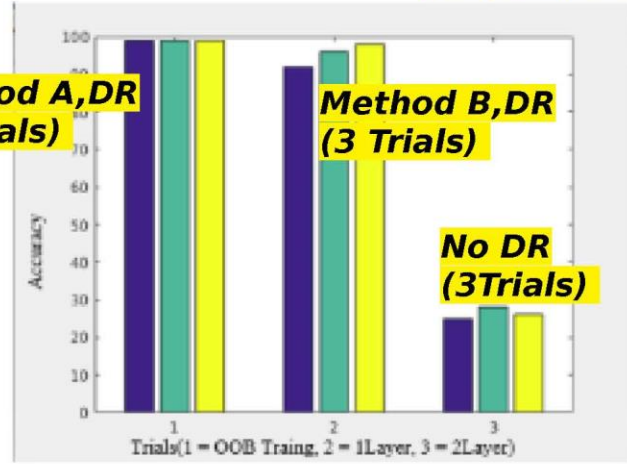
- Autoencoder(AE) learns a reduced manifold model of the input features

- Classifies with a reduced set of features and reduced computational time

Future Work:

- Coupling ML methods with finite difference time domain (FDTD) plasmonic simulation methods (See Projects 1 and 2)

- Characterization and prediction of the response of the heterogeneous nanostar substrate morphology to photonic excitation without computationally expensive FDTD simulation of substrate



Research - Project 5: Predicting Quantum Mechanical Properties of Molecular Structures Utilizing Density Functional Theory and High Performance Computing

Luis Garcia
BS CS, NMHU

4th Semester Graduate Student , MS CS, NMHU

Research: Computational modeling/ simulation of metamaterials and AI/machine learning and HPC

Employment: LANL

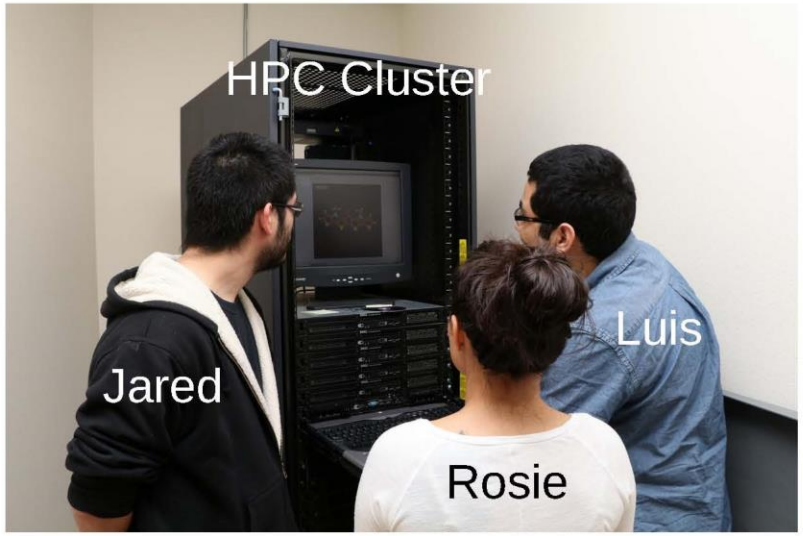
- Predict quantum mechanical properties of molecular structure

- Simulation complex molecules using DFT calculations on a HPC system

- Two parallel computing HPC clusters running Gauss and CUDA

- The primary goal of this research is to improve the computational efficiency of the DFT calculations, while ensuring the accuracy is not lost

- Future work will be to construct features and labels for machine learning and predict quantum mechanical properties using an ANN



Cluster	GPU Cores	CPU Cores	OS
Xeon,2- Nvidia Tesla K80	~10000	3	Redhat
Xeon, 2-Nvidia Tesla K10	~7000	3	Redhat

Research – Other Projects

- Development of a novel machine learning methods to take SEM images and EM simulations to generate features and labels for an ANN to train on for prediction of novel SEM image EM response.
- Co-authored and published one refereed paper in IEEE journal related to machine learning and plasmonic biosensors for detection of early onset Alzheimer's Disease.

Education

- Course Development:

  - Data Science I, Data Science II, Machine Learning, Artificial Neural Networks, Artificial Intelligence, Cognitive Science have been offered since 2015 as part of the support for AI and Machine Learning in computer science as it relates to many science disciplines. These courses all included materials science related problems to emphasize the importance in this field.

  - A Machine Learning Short Course was taught by experts in industry to twenty undergraduate and graduate students during the summer of 2016. Each student was able to develop skills in solving problems in materials science related to biosensor design utilizing the latest method in machine learning.

Role of the partnering institution

- Three undergraduate students, Jason Marquez, Patricio Herrera and Taylor Herrera worked in three groups at OSU during the summers from 2017-18. They worked on modeling magnetic materials systems with several of our colleagues at OSU.